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Title: Report for computational project w19_ionpolymers (2nd year) Computationally Assisted Design of Ion-conducting Polymers for Anion Exchange Membrane Fuel Cells

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Computationally Assisted Design of Ion-conducting Polymers for Anion Exchange Membrane Fuel Cells

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Phosphonated polymers have been proposed as proton conductors for fuel cells; however, the anhydride formation of phosphonic acid functional groups lowers proton conductivity and hinders their use in fuel cell applications. We used calculations to support this hypothesis by correlating calculated Gibbs free energies for the formation of the anhydride with pK values of the corresponding acid. The results showed that stronger acids are less likely to form an anhydride even at elevated temperatures and *supported the design of a new polymer and the high-temperature proton exchange membrane fuel cell (HT-PEMFC) that outperformed other state-of-the-art* HT-PEMFCs.

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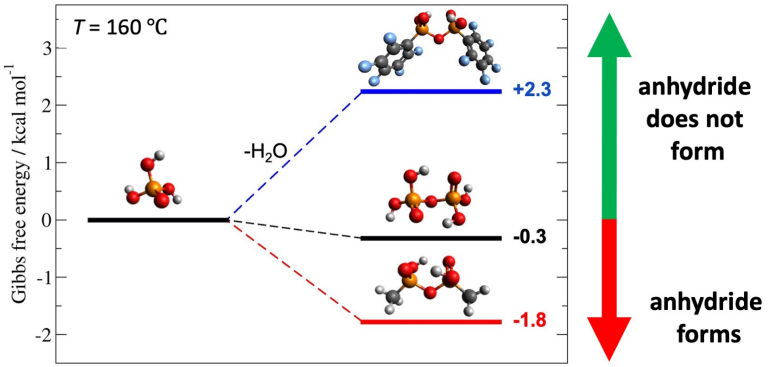

Figure 1. Gibbs free energy for the formation of an anhydride from an acid for three acids with different pK at 160 °C. Anhydride formation is detrimental in working HT-PEMFCs.

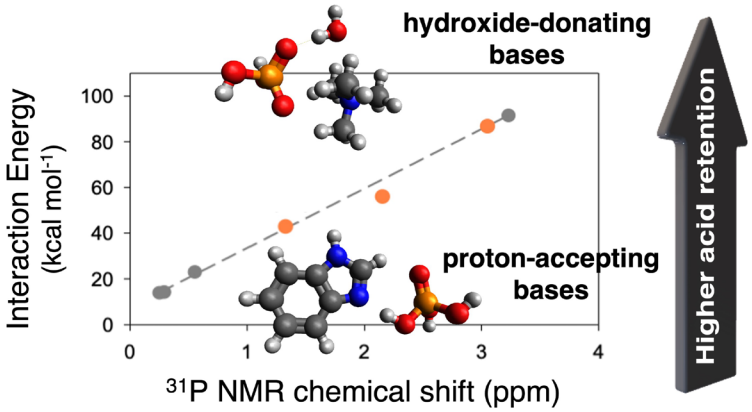

Figure 2. Higher interaction energy between phosphoric acid and hydroxide-donating group in the polymer leads to less acid leaching and higher stability of the HT-PEMFC.

The interaction energy of base−acid plays a key role in acid retention of phosphoric acid-doped polymer electrolytes under HT-PEMFC operating conditions. We used density functional theory calculations to investigate the energetics of phosphoric acid (PA) and proton-accepting and hydroxide-donating organic bases, which are used in the design of polymer electrolytes for HT-PEMFCs. The results show that because of their weak basicity, proton-accepting organic bases have relatively low interaction energy (15.3−28.0 kcal mol^{-1}) while hydroxide-donating organic bases have high interaction energy with PA (~110 kcal mol^{-1}), which remains high in the presence of water. These results *revealed benefits of incorporating hydroxide-donating organic bases into the polymer electrolyte as a way to increase the stability of the HT-PEMFCs.*

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